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1 Introduction

This note provides a summary of what isotopes and nuclear reaction chains would be of interest to astrophysicists using FLAG. It is meant to suggest nuclear data and nuclear burning networks that could be added to FLAG's default libraries to make it a more attractive code option for astronomers.

Astrophysics simulations cover a huge variety of situations and temperature/density regimes, far more than a single note can discuss. Instead I will focus on two subfields that involve substantial nuclear reaction calculations: stellar evolution and supernovae. These are not the only scenarios that use nuclear reaction networks, but both are major problems with numerous researchers working on them.

Astrophysics simulations use two types of nuclear reaction networks: fusion-centered energy-generating ones, and detailed nucleosynthetic ones. Energy-generating networks are used to model the fusion processes that support a star against gravity while nucleosynthetic ones follow the creation of new isotopes in stars and stellar explosions. Fusion networks usually have 10-20 different isotopes and are relatively simple to solve. Following detailed nucleosynthetic processes, on the other hand, requires complex reaction networks that track huge numbers of isotopes and reactions. These processes contribute little in the way of energy but greatly affect the chemical outcome. Rather than build such complex networks from scratch, astronomers often use open-source reaction libraries like Reaclib or SkyNet (co-authored by LANL scientist Jonas Lippuner) none of which are currently compatible with FLAG.

The elements most commonly used in astrophysics simulations are hydrogen, helium, carbon, oxygen, neon, silicon, magnesium, iron, and associated iron-peak elements. Some simplify this mix further to hydrogen (denoted X), helium (Y), and "metals" (all other elements, Z (not to be confused with redshift z)). Some consider radioactive isotopes neglected in other areas because of their short lifetimes, as their decay powers observable signals; for supernova research the isotopes ^{56}Ni and ^{56}Co and their decay chain are especially important.

Isotopic composition, as opposed to just elemental, is important for two types of physics: nuclear reaction networks and atomic weight. The details of atomic weight are mostly only relevant to precise opacity calculations, which FLAG cannot currently make, and 3T calculations, which FLAG does make. With its current radiation physics FLAG cannot model frequency-dependent radiation at all, let alone resolve the kind of line-splitting that would distinguish isotopes. Isotope details are also relevant to the electron/ion splits for 3T calculations, but even if a given isotope is not in FLAG's default library, the user should be able to proceed by substituting another. Using the wrong isotope might skew the atomic weight, but as long as one of similar A is substituted, the resulting error should be minimal. The remainder of this note will therefore consider only the nuclear burning case.

Since nuclear reaction network calculations consume plenty of resources, no one wants to carry more isotopes than necessary; hence astrophysicists have converged on several standard networks that use as few isotopes & reactions as possible while still producing the right net energy and nucleosynthesis. Astrophysicists also often take models produced by one code and map them into another to run different calculations, and this mapping is much easier when the two codes share an isotopic network. It's therefore worth considering not only what elements are necessary for research, but also what the most common networks are and how easily they could be added to FLAG.

2 Stellar Evolution

Stellar evolution models simulate a star's life from (just after) beginning to (nearly) end. Stars spend most of their life on the "main sequence," steadily fusing hydrogen into helium as their primary power source. Once central hydrogen is exhausted most stars will proceed to helium burning. After central helium exhaustion, massive stars ($\geq$ 8 $M_{\odot}$) will continue on to heavier fusion stages, burning carbon, oxygen, and silicon before dead-ending at iron. Though central fusion reactions provide most of the star's supporting energy, during helium-burning and beyond multiple fusion processes will occur simultaneously in shells of material surrounding the core. Therefore, the heavier the star and the further in its life it is followed, the larger the reaction network needs to be to encompass all relevant reaction chains.

During the hydrogen burning (main sequence) phase of a star's life, fusion proceeds along two chains: the proton-proton chain ("pp chain"), which provides the main source of energy in stars about the same mass as our Sun; and the "cold" or β-limited carbon-nitrogen-oxygen cycle ("β-limited CNO"), which dominates energy production in massive stars. Post-main-sequence, the most common reaction chain considered is the α-chain, which starts with a ^{4}He nucleus and keeps adding α particles until it reaches the nuclear density peak around iron. A massive star evolving post-main-sequence will pass through four distinct central fusion stages: helium burning, carbon burning, oxygen burning, and finally silicon burning. As a rule of thumb, the more massive the star, the shorter it lives. Our Sun, an average star, has a hydrogen-burning lifespan of about ten billion years while a massive star like Betelgeuse will consume its central hydrogen in only a few million. Each subsequent burning stage proceeds exponentially faster than the previous one; helium burning lasts on order a few hundred thousand years while silicon burning is over in a day. During each of these stages it can be assumed that all lighter reactions are still proceeding in shells of material around the core, giving the final star a distinct "onion" structure of concentric, increasingly-heavy elemental layers.

2.1 Post-Main-Sequence Fusion

Central helium burning begins with the triple-α reaction, $3\alpha \rightarrow ^{12}$C, and transitions to the ^{12}C + $\alpha \rightarrow$ ^{16}O reaction as α abundance drops and carbon rises. There is no hard transition point between the two and this fusion stage leaves behind well-mixed carbon and oxygen ash. As a result the final core produced is just called the "carbon-oxygen core" and considered as a single unit. At this point degeneracy pressure will also begin to play a significant role in supporting the star against collapse. In lower-mass stars fusion ends here and the star will eventually expel its leftover hydrogen envelope as a planetary nebula, leaving behind a compact CO white dwarf core.

Central carbon burning ignites after further contraction. Carbon prefers to react with itself as ^{12}C + ^{12}C, with a multitude of possible outcomes. The two most common products are ^{23}Na + p and ^{20}Ne + α. The proton liberated by the first reaction captures onto another ^{12}C nucleus to form ^{13}N, which decays back down to ^{13}C and then picks up an alpha particle to produce ^{16}O + n. This chain is an important source of free neutrons for later nucleosynthesis. The free α particles from the second reaction will capture onto available nuclei to form ^{16}O, ^{20}Ne, ^{24}Mg, and ^{28}Si. Some stars will cease fusion here, eventually producing a planetary nebula and a heavier O-Ne-Mg white dwarf. Otherwise, after a brief neon-burning phase only important to nucleosynthesis, central oxygen burning ignites. Oxygen, like carbon, prefers to react with itself as ^{16}O + ^{16}O and proceeds through multiple channels, primarily ^{32}S + γ and ^{28}Si + α. This stage produces several elements but the primary end-product is ^{28}Si with some ^{32}S.

At first glance it might seem like magnesium burning should come next. However the ^{24}Mg + ^{24}Mg reaction turns out to require staggeringly high temperatures, and before the star heats up enough photodisintegration rearrangement of ^{28}Si and ^{32}S nuclei will begin instead. This phase is called "silicon burning" but is really more like "silicon melting." Photodisintegration rearrangement is a messy process where nuclei are repeatedly split apart by extremely-high-energy photons and recombine in various proportions. Ultimately, however, these reactions will seek the lowest-energy state: the iron peak around ^{56}Fe and ^{56}Ni, where the maximum possible binding energies are found. This process is throttled by the photodisintegration rate of ^{28}Si, the more tightly-bound of the two nuclei, and is usually summarized by ^{28}Si + ^{28}Si $\rightarrow$ ^{56}Ni and/or ^{28}Si

+ ^{28}Si $\rightarrow$ ^{54}Fe + $2p$, depending on temperature.

If the simulated star is being modeled for ultimate use as a supernova progenitor, the user may want to track additional isotopes that have little impact during the star's lifetime but affect nucleosynthesis during the supernova. Red giant stars of a particular age and mass, called asymptotic giant branch (AGB) stars, are also the site of important nucleosynthesis and need their chemical composition well-modeled throughout when studying these processes. See Section 4.1 for additional information on these networks.

2.2 Recommended Networks

The basic reactions of stellar evolution can be captured by a minimal set of isotopes. The most commonly-used are:

Basic α-chain, 13-isotope network: {^{4}He, ^{12}C, ^{16}O, ^{20}Ne, ^{24}Mg, ^{28}Si, ^{32}S, ^{36}Ar, ^{40}Ca, ^{44}Ti, ^{48}Cr, ^{52}Fe, ^{56}Ni} Captures post-main-sequence evolution. This network implicitly includes ^{27}Al, ^{31}P, ^{35}Cl, ^{39}K, ^{42}Sc, ^{47}V, ^{51}Mn, and ^{55}Co as intermediate isotopes whose fractions can be determined by assuming the reactions are in steady-state.

The α-chain plus the pp chain and the CNO cycle, 18-isotope network: {^{1}H, ^{3}He, ^{4}He, ^{12}C, ^{14}N, ^{16}O, ^{20}Ne, ^{24}Mg, ^{28}Si, ^{32}S, ^{36}Ar, ^{40}Ca, ^{44}Ti, ^{48}Cr, ^{52}Fe, ^{56}Ni} Captures main sequence and post-main-sequence evolution. Supernova calculations add ^{54}Fe to account for photodisintegration of iron during the explosion.

The α-chain, pp chain, CNO cycle, photodisintegration processes, plus the isotopes ^{56}Cr and ^{56}Fe for calculating exact electron fractions: {^{1}H, ^{3}He, ^{4}He, ^{12}C, ^{14}N, ^{16}O, ^{20}Ne, ^{24}Mg, ^{28}Si, ^{32}S, ^{36}Ar, ^{40}Ca, ^{44}Ti, ^{48}Cr, ^{56}Cr, ^{52}Fe, ^{54}Fe, ^{56}Fe, ^{56}Ni} This 21-isotope network sees widespread use as the current default in the popular open-source stellar evolution code MESA.

FLAG's current hydro is not sufficiently implicit to handle stellar evolution simulations, which need to take timesteps of order thousands to hundreds of thousands of years. But since models produced by stellar evolution codes are often mapped into other codes for further simulation, FLAG would benefit from being able to easily instantiate these networks.

3 Supernova Simulations

The most important isotopes needed in supernova calculations are the radioactive ones that power the event's overall observable light curve. Core-collapse supernovae radiate large amounts of light from hydrogen recombination; Type Ia supernovae, lacking a hydrogen envelope, have light curves powered entirely by radioactive decay. Initially the energy comes from β decay of ^{56}Ni into ^{56}Co, shifting after several days to β decay of ^{56}Co into ^{56}Fe and after several months to decay of ^{44}Ti into ^{44}Sc.

3.1 Core-Collapse Supernovae

Core-collapse supernovae (CCSNe) occur when a massive star fuses its core material all the way up to iron. Since iron sits at the peak of the nuclear density curve, fusing iron costs energy rather than yielding it. As the fusion energy supporting it drains away, gravity will finally overcome pressure and the star will begin to implode, eventually hitting central densities so great that the iron core collapses into a neutron star. When this happens the star's implosion becomes an explosion and a core-collapse supernova occurs. A CCSN is over in hours, a day at most, but produces a tremendous amount of nucleosynthesis in that time.

As the shock wave propagates outwards through the star it causes a great deal of photodisintegration and explosive burning reactions. ^{56}Ni is a doubly-magic nucleus, having 28 protons and 28 neutrons. Reacting nuclei would really, really like to be ^{56}Ni, and the tremendous temperatures and densities in the shock wave of a CCSN will give many of them that chance. A star that begins its life at 15 $M_{\odot}$ will produce about a tenth of a solar mass of ^{56}Ni when it explodes, and the vast majority of that material will be produced during the supernova itself as the pre-existing iron core either collapses into the neutron star or gets photodisintegrated during the explosion. A modified version of the CNO cycle, called the "hot CNO cycle" or "non-β-limited CNO cycle," occurs at these extreme temperatures and following this process accurately requires adding ^{14}N to the suite of CNO isotopes. The rp-process, γ-process. and ν-process also happen during the CCSN itself, though they'll be discussed in Section 4.

Many large networks for extreme conditions ($T \geq 5 \times 10^9$ K) handle hundreds of isotopes by assuming nuclear statistical equilibrium i.e. forward and reverse reaction rates have balanced out. However, these networks can't always be used when a CCSN calculation is tracking the shockwave. Some of the stellar material will undergo "freezeout" as the explosive shockwave heats and compresses it just long enough to start reaction chains but not long enough for isotopic fractions to equilibrate. Supernova shocks tend to produce α-rich freezeout in which a number of α particles are knocked free but don't have time to recombine before the shockwave moves on. Because tracking freezeout requires actual tracking of reactions instead of assuming NSE, these shock calculations can get very expensive very quickly.

3.2 Type Ia Supernovae

Type Ia supernovae differ substantially from CCSNe. These events are caused by the collapse and detonation of a white dwarf that has exceeded the Chandrasekar mass, the maximum possible mass supportable by electron degeneracy. Though astronomers still debate exactly how said white dwarf gains enough mass to ignite, all models start as a compact CO or O-Ne-Mg object with little to no hydrogen or helium. As a result the supernova has no large, ionized envelope to produce light via recombination and all power in its light curve must come from radioactive decay of newly-synthesized elements.

Type Ia supernovae are the primary source of iron-peak elements in the universe and were thought to be the site of the r-process, though more recent data prefers merging neutron stars; they are also the subject of intense research due to their importance as standard candles in cosmology. Astronomical distances are surprisingly hard to measure. In order to distinguish between a bright object far away and a dim object nearby, astronomers use "standard candles," objects whose intrinsic brightness can be found from other observable quantities. The intrinsic brightness can then be compared to the observed brightness to determine the distance to that object and by extension its surroundings. Individual stars are used for distances on the scale of the Milky Way and its neighbors, but on cosmic scales these objects are far too dim.

Type Ia SNe are some of the brightest events in the universe and, more importantly, their intrinsic brightness can be determined solely by observation. A Type Ia supernova's peak brightness is directly related to the light curve duration because both are determined by the mass of radioactive ^{56}Ni produced in the explosion. The exact function that relates the two, called the Phillips relation, is calibrated & refined via simulation. This relation plus observations of Type Ia SNe allowed astronomers to measure precise galactic distances on previously unreachable scales, work that led directly to the discovery of the accelerating expansion of the universe and the theory of dark energy (and the 2011 Nobel Prize in Physics). Dark energy and expansion cosmology are fields of active research and predictions of the ^{56}Ni yield from different events are always in demand. Astronomers still run dozens of large-scale simulations on the subject every year. If FLAG implemented the capabilities necessary to accurately model the final mass of ^{56}Ni and its decay, we could expect it to be used for that purpose for a long time.

3.3 Recommended Networks

From a nuclear burning standpoint, modeling the basics of supernovae and their light curves requires first and foremost the addition of the processes that produce ^{56}Ni, and later the $^{56}\text{Ni} \rightarrow {}^{56}\text{Co} \rightarrow {}^{56}\text{Fe}$ decay chain. Much of the radioactive material from CCSNe is produced in the explosive burning stage, so these simulations need a network that accounts for photodisintegration at shockwave temperatures/densities as well as nuclear freezeout.

4 Nucleosynthesis

Some stellar evolution and supernova simulations are run not only to follow the behavior of the star but also to model the nucleosynthesis, the overall production of chemical elements. The vast majority of isotopes heavier than lithium in the universe are created in stars, supernovae, or compact object mergers. A full description of all nucleosynthetic processes could (and does) fill multiple textbooks; this note will attempt to give a summary focused on the networks themselves. Nucleosynthetic networks need to follow far more isotopes than networks focused on energy generation, and as a result can quickly become enormous. For example, one network handling only the weak s-process has 341 isotopes linked by 3394 reactions; another network extending only to germanium (Z=32) still has 200 isotopes.

4.1 The s-process and AGB Stars

The most complex nucleosynthetic process likely to be studied during a star's lifetime, as opposed to during a supernova event, is the "slow process" or s-process. It produces a huge chunk of the periodic table - nearly all chemical isotopes from $56 < A < 204$ - and proceeds via neutron capture followed by inverse β-decay in an environment where free neutron capture happens far slower than the lifetimes of the unstable isotopes (hence "slow process"). A stable s-process nucleus will capture free neutrons until it reaches an unstable isotope, then decay back to stability by converting neutrons to protons. This allows nuclei to steadily climb in Z well past the iron peak where central fusion stops.

The s-process comes in two flavors: the main s-process ($90 < A < 204$), which occurs in red giant stars and produces most isotopes, and the weak s-process ($56 < A < 90$), which happens during core helium burning and produces extra amounts of nuclei around the Sr-Y-Zr peak. There is no difference in the actual mechanism of the two, but the weak s-process requires seed iron peak nuclei, meaning at least one local generation of Type Ia SNe must have already formed and exploded. In this manner the excess abundances in the Sr-Y-Zr peak can be used to estimate ages of galaxies.

The main s-process site in the universe is red giant stars of a particular age and mass range (0.5 - 10 $M_\odot$), called asymptotic giant branch (AGB) stars. These stars have already completed central hydrogen and helium burning, creating a large CO core surrounded by layered helium and hydrogen. They will undergo a few dozen slow pulsations in brightness, each lasting a few thousand years, caused by periodic runaway fusion in helium shells. During these phases of intense helium fusion the temperatures, densities, and free neutron abundance reach levels high enough to start the s-process. Modeling runaway shell burning directly is beyond the reach of most stellar evolution codes, as it requires detailed convection analysis, but simplified prescriptions exist that simply tell the code to start the s-process when other state variables are in a certain range.

Free neutron abundance limits the s-process. For the main s-process neutrons come from the reaction $^{13}\mathrm{C} + \alpha \rightarrow {}^{16}\mathrm{O} + \mathrm{n}$ (see Section 2.1). For the weak s-process neutrons come from neon burning via $^{22}\mathrm{Ne} + \alpha \rightarrow {}^{25}\mathrm{Mg} + \mathrm{n}$. Since these two reactions produce little energy, fusion-centered networks will neglect them, but a simulation interested in the s-process must follow them at early times to track neutron abundance later on. The s-process terminates at the reaction cycle $^{209}\mathrm{Bi} \rightarrow {}^{210}\mathrm{Po} \rightarrow {}^{206}\mathrm{Pb} \rightarrow {}^{209}\mathrm{Pb} \rightarrow {}^{209}\mathrm{Bi}$, where decay and formation rates balance out.

4.2 r-process

The site of the "rapid process" or r-process is still a matter of debate, but recent gravitational wave observations have tipped the balance strongly in favor of compact object mergers. Compact objects are defined as white dwarfs (objects supported by electron degeneracy pressure), neutron stars (pure neutronic material supported by neutron degeneracy pressure), or black holes; the r-process in particular seems to occur in mergers of two neutron stars. Most matter in the initial compact objects will end up in the combined neutron star or a new black hole, but during the merger angular momentum conservation will expel a large tail of processed material. In this environment temperatures and densities are high, entropy is high, and free neutron abundance is *very* high, allowing unstable isotopes to quickly capture neutrons before they decay (hence "rapid process"). Isotopes in this environment will capture neutrons up to the neutron drip line, the energetic "break-even" point where no more can be crammed into the nucleus, before returning to the valley of stability via inverse beta decay. Since the surplus of neutrons will decay into protons, the r-process can skip past the termination point of the s-process and reach far higher Z numbers. The r-process produces nearly all platinum-group isotopes plus the highest-Z elements up to the natural upper limit at uranium.

4.3 rp-process

The rp-process is named in analogy to the r-process since it proceeds via the same mechanism except with protons instead of neutrons. The proton's charge, however, means that this process requires far higher temperatures ($\sim 10^9$) to overcome the Coulumb barrier, and thus it happens far less often. It produces proton-rich isotopes up to ^{105}Te, where the α decay rate balances it out.

4.4 γ-process

The γ process occurs only in explosive burning during core-collapse supernovae and produces proton-rich isotopes via photodisintegration of s- and r-process nuclei. Gamma rays knock neutrons, protons, or full α particles out of the seed nuclei, which then decay back to stability if necessary. It can only occur during an explosive burning phase both because of the immense temperatures required and because of the very short timescale, which keeps the photons from disintegrating the nuclei entirely.

4.5 ν-process

Similar to the γ process, the ν-process involves the spallation of heavier nuclei, in this case by neutrinos. Since the interaction cross-sections are so low this process requires an extraordinarily high density of both matter and neutrinos, and happens only in the opening stages of a core-collapse supernova when the overlying matter of the star is briefly illuminated by the incredible neutrino flux emitted by the newly-formed neutron star at the core. It produces a number of oddball isotopes missed by other processes, usually because a much more stable isotope is right next door. ^{7}Li, ^{11}B, ^{138}La, ^{180}Ta, ^{22}Na, ^{26}Al, and ^{19}F are all made by this process - so you have neutrinos to thank the next time you brush with flouride toothpaste.

5 Summary

The most important isotopes to add to the FLAG data libraries are ^{56}Ni, ^{56}Co, and to a lesser extent ^{44}Ti. The library does not include these isotopes by default because their relatively short half-lives mean they do not occur on Earth in measurable quantities. However, they occur in large quantities in an astrophysical context. The decay of these isotopes is the main power source for supernova light curves and modeling the quantity produced and their distribution & mixing is critical in connecting simulations to observable results. Astronomers also need information on noble gases not often included because of their minimal reactivity.

The reaction networks described in this note are all common networks used in many open-source astrophysics codes. The data on reaction rates, equilibrium, etc. are publicly available and widely distributed. In the long term FLAG will benefit greatly from having an interface to ReacLib, an open-source astrophysics library of nuclear data. All information in ReacLib is publicly available and has been used in published results computed with large-scale astrophysics codes such as CASTRO and FLASH, often in 3D with neutrino transport and other effects.

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